A Concise Formula for Generalized Two-Qubit Hilbert-Schmidt Separability Probabilities

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(Dated: January 29, 2013)

Abstract

We report major advances in the research program initiated in "Moment-Based Evidence for Simple Rational-Valued Hilbert-Schmidt Generic 2×2 Separability Probabilities" (*J. Phys. A*, **45**, 095305 [2012]). A function $P(\alpha)$, incorporating a family of six hypergeometric functions, all with argument $\frac{27}{64} = (\frac{3}{4})^3$, is obtained. It reproduces a series, $\alpha = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots, 32$, of sixty-four conjectured Hilbert-Schmidt rational-valued generic 2×2 separability probabilities. These exact ratios are put forth on the basis of systematic, high-accuracy probability-distribution-reconstruction computations, employing 7,501 determinantal moments of partially transposed 4×4 density matrices. A lengthy expression for $P(\alpha)$ containing six generalized hypergeometric functions is initially obtained–making use of the FindSequenceFunction command of Mathematica. A remarkably succinct reexpression for $P(\alpha)$ is then found, by Qing-Hu Hou and colleagues, using Zeilberger's algorithm ("creative telescoping"), For generic (9-dimensional) two-rebit systems, $P(\frac{1}{2}) = \frac{29}{64}$, (15-dimensional) two-qubit, $P(1) = \frac{8}{33}$ (a value that had been proposed in *J. Phys. A*, **40**, 14279 [2007] and supported in *Intl. J. Mod. Phys. B*, **26**, 1250054 [2012]) and (27-dimensional) two-quater(nionic)bit systems, $P(2) = \frac{26}{323}$.

PACS numbers: Valid PACS 03.67.Mn, 02.30.Zz, 02.30.Gp

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I. INTRODUCTION

The predecessor paper [1]–addressing the relatively long-standing 2×2 separability probability question [2–11] (cf. [12–14])–consisted largely of two sets of analyses. (In the foundational study [2], "three main reasons of importance"–philosophical, practical and physical–were given for studying this question.) The first set of analyses in [1] was concerned with establishing formulas for the bivariate determinantal product moments $\left\langle \left|\rho^{PT}\right|^n |\rho|^k \right\rangle, k, n = 0, 1, 2, 3, \ldots$, with respect to Hilbert-Schmidt (Euclidean/flat) measure [15] [16, sec. 14.3], of generic (9-dimensional) two-rebit and (15-dimensional) two-qubit density matrices (ρ). Here ρ^{PT} denotes the partial transpose of the 4×4 density matrix ρ. Nonnegativity of the determinant $|\rho^{PT}|$ is both a necessary and sufficient condition for separability in this 2×2 setting [17].

In the second set of analyses in [1], the *univariate* determinantal moments $\left\langle \left|\rho^{PT}\right|^n \right\rangle$ and $\left\langle \left(\left|\rho^{PT}\right| |\rho|\right)^n \right\rangle$, induced using the bivariate formulas, served as input to a Legendre-polynomial-based probability distribution reconstruction algorithm of Provost [18, sec. 2] (cf. [19]). This yielded estimates of the desired separability probabilities. (The reconstructed probability distributions based on $|\rho^{PT}|$ are defined over the interval $|\rho^{PT}| \in [-\frac{1}{16}, \frac{1}{256}]$, while the associated separability probabilities are the cumulative probabilities of these distributions over the nonnegative subinterval $|\rho^{PT}| \in [0, \frac{1}{256}]$. We note that for the fully mixed (classical) state, $|\rho^{PT}| = \frac{1}{256}$, while for a maximally entangled state, such as a Bell state, $|\rho^{PT}| = -\frac{1}{16}$.)

A highly-intriguing aspect of the (not yet rigorously established) determinantal moment formulas obtained (by C. Dunkl) in [1, App.D.4] was that both the two-rebit and two-qubit cases could be encompassed by a *single* formula, with a Dyson-index-like parameter α [20] serving to distinguish the two cases. The value $\alpha = \frac{1}{2}$ corresponded to the two-rebit case and $\alpha = 1$ to the two-qubit case. (Let us note that the results of the formula for $\alpha = 2$ and $n = 1$ and 2 have recently been confirmed computationally by Dunkl using the "Moore determinant" (quasideterminant) [21, 22] of 4×4 quaternionic density matrices. However, tentative efforts of ours to verify the $\alpha = 4$ [conjecturally, *octonionic* [23], problematical] case, have not proved successful.)

When the probability-distribution-reconstruction algorithm [18] was applied in [1] to the two-rebit case ($\alpha = \frac{1}{2}$), employing the first 3,310 moments of $|\rho^{PT}|$, a (lower-bound) estimate

that was 0.999955 times as large as $\frac{29}{64} \approx 0.453120$ was obtained (cf. [24, p. 6]).

Analogously, in the two-qubit case ($\alpha = 1$), using 2,415 moments, an estimate that was 0.999997066 times as large as $\frac{8}{33} \approx 0.242424$ was derived. This constitutes an appealingly simple rational value that had previously been conjectured in a quite different (non-moment-based) form of analysis, in which "separability functions" had been the main tool employed [11]. (Note, however, that the the two-rebit separability probability conjecture of $\frac{8}{17}$, somewhat secondarily advanced in [11], has now been discarded in favor of $\frac{29}{64}$.) Let us, importantly, note that in an extensive Monte Carlo analysis, Zhou, Chern, Fei and Joynt obtained an estimate for this two-bit separability probability of 0.2424 ± 0.0002 [25, eq. (B7)], thus, fully consistent with our exact proposal.

Further, the determinantal moment formulas advanced in [1] were then applied with α set equal to 2. This appears–as the indicated recent (Moore determinant) computations of Dunkl show–to correspond to the generic 27-dimensional set of quaternionic density matrices [26, 27]. Quite remarkably, a separability probability estimate, based on 2,325 moments, that was 0.999999987 times as large as $\frac{26}{323} \approx 0.0804954$ was found. (In line with this set of three results, the paper [1] was entitled, "Moment-Based Evidence for Simple Rational-Valued Hilbert-Schmidt Generic 2×2 Separability Probabilities".)

In the present study, we extend these three (individually-conducted) moment-based analyses in a more systematic, thorough manner, *jointly* embracing the sixty-four integral and half-integral values $\alpha = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots, 32$. We do this by accelerating, for our specific purposes, the Mathematica probability-distribution-reconstruction program of Provost [18], in a number of ways. Most significantly, we make use of the three-term recurrence relations for the Legendre polynomials. Doing so obviates the need to compute each successive higher-degree Legendre polynomial *ab initio*.

In this manner, we were able to obtain–using exact computer arithmetic throughout–"generalized" separability probability estimates based on 7,501 moments for $\alpha = \frac{1}{2}, 1, \frac{3}{2}, \ldots, 32$. In Fig. 1 we plot the logarithms of the resultant sixty-four separability probability estimates (cf. [1, Fig. 8]), which fall close to the line -0.9464181889α. In Fig. 2 we show the residuals from this linear fit.

In Fig. 3 we present a hypergeometric-function-based formula, together with striking supporting evidence for it, that appears to succeed in uncovering the functional relation ($P(\alpha)$) underlying the entirely of these sixty-four generalized separability probabilities. Further, in

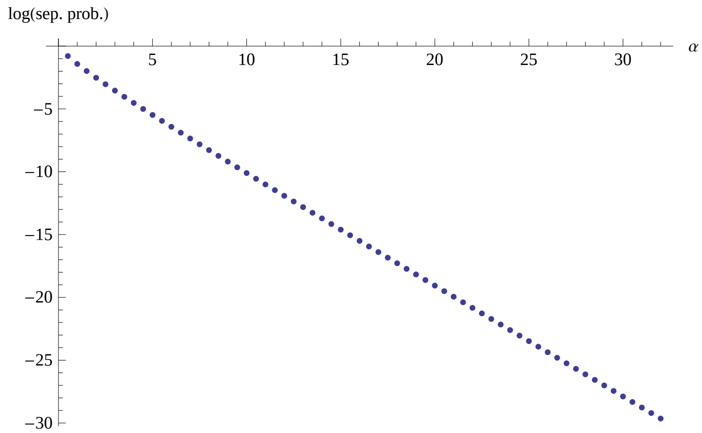

FIG. 1: Logarithms of generalized separability probability estimates, based on 7,501 Hilbert-Schmidt moments of $|\rho^{PT}|$, as a function of the Dyson-index-like parameter α

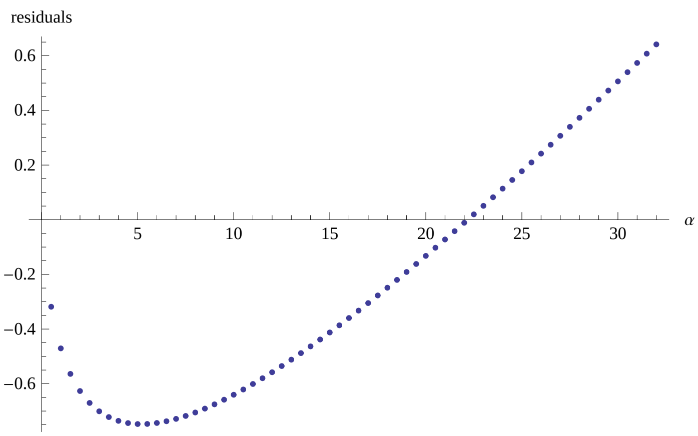

FIG. 2: Residuals from linear fit to logarithms of generalized separability probability estimates

(3), and the immediately preceding text, we list a number of remarkable values yielded by this hypergeometric formula for values of α other than the basic sixty-four (half-integral and integral) values from which we have started.

Then, we are able to report–with the assistance of Qing-Hu Hou and colleagues–of a remarkable condensation of the lengthy expression presented in Fig. 3.

In[3]:= **TraditionalForm[formula]**

Out[3]//TraditionalForm=

$$\Bigg(4^{-2\alpha-3}\,\Gamma\!\left(3\alpha+\frac{5}{2}\right)\Gamma(5\alpha+2)\Bigg(\Big(\alpha(5\alpha(25\alpha(2\alpha(740\alpha-581)+161)+628)+39)-54\Big)\,{}_7F_6\!\left(1,\alpha+\frac{2}{5},\alpha+\frac{3}{5},\alpha+\frac{4}{5},\alpha+\frac{5}{6},\alpha+\frac{7}{6},\alpha+\frac{6}{5};\alpha+\frac{13}{10},\alpha+\frac{3}{2},\alpha+\frac{17}{10},\alpha+\frac{19}{10},\alpha+2,\alpha+\frac{21}{10};\frac{27}{64}\right)+(5\alpha(25\alpha(8\alpha(925\alpha-2431)+22255)-312019)+347274)\,{}_7F_6\!\left(2,\alpha+\frac{2}{5},\alpha+\frac{3}{5},\alpha+\frac{4}{5},\alpha+\frac{5}{6},\alpha+\frac{7}{6},\alpha+\frac{6}{5};\alpha+\frac{13}{10},\alpha+\frac{3}{2},\alpha+\frac{17}{10},\alpha+\frac{19}{10},\alpha+2,\alpha+\frac{21}{10};\frac{27}{64}\right)+10\Bigg((25\alpha(4\alpha(3700\alpha-12843)+66227)-769797)\,{}_7F_6\!\left(3,\alpha+\frac{2}{5},\alpha+\frac{3}{5},\alpha+\frac{4}{5},\alpha+\frac{5}{6},\alpha+\frac{7}{6},\alpha+\frac{6}{5};\alpha+\frac{13}{10},\alpha+\frac{3}{2},\alpha+\frac{17}{10},\alpha+\frac{19}{10},\alpha+2,\alpha+\frac{21}{10};\frac{27}{64}\right)+75\Bigg((8\alpha(1850\alpha-6131)+44133)\,{}_7F_6\!\left(4,\alpha+\frac{2}{5},\alpha+\frac{3}{5},\alpha+\frac{4}{5},\alpha+\frac{5}{6},\alpha+\frac{7}{6},\alpha+\frac{6}{5};\alpha+\frac{13}{10},\alpha+\frac{3}{2},\alpha+\frac{17}{10},\alpha+\frac{19}{10},\alpha+2,\alpha+\frac{21}{10};\frac{27}{64}\right)+8\Bigg((3700\alpha-7981)\,{}_7F_6\!\left(5,\alpha+\frac{2}{5},\alpha+\frac{3}{5},\alpha+\frac{4}{5},\alpha+\frac{5}{6},\alpha+\frac{7}{6},\alpha+\frac{6}{5};\alpha+\frac{13}{10},\alpha+\frac{3}{2},\alpha+\frac{17}{10},\alpha+\frac{19}{10},\alpha+2,\alpha+\frac{21}{10};\frac{27}{64}\right)+3700\,{}_7F_6\!\left(6,\alpha+\frac{2}{5},\alpha+\frac{3}{5},\alpha+\frac{4}{5},\alpha+\frac{5}{6},\alpha+\frac{7}{6},\alpha+\frac{6}{5};\alpha+\frac{13}{10},\alpha+\frac{3}{2},\alpha+\frac{17}{10},\alpha+\frac{19}{10},\alpha+2,\alpha+\frac{21}{10};\frac{27}{64}\right)\Bigg)\Bigg)\Bigg)\Bigg)\Bigg)\Bigg/\left(3\,\Gamma(\alpha+1)\,\Gamma(2\alpha+3)\,\Gamma\!\left(5\alpha+\frac{13}{2}\right)\right)$$

In[4]:= **N[formula /. α → 1 / 2, 100] / (29 / 64)**

Out[4]= 1.0000000000000000000000000000000000000000000000000000000000000000000000000000000000000\
00000000000000

In[5]:= **N[formula /. α → 1, 100] / (8 / 33)**

Out[5]= 1.0000000000000000000000000000000000000000000000000000000000000000000000000000000000000\
00000000000000

In[6]:= **N[formula /. α → 2, 100] / (26 / 323)**

Out[6]= 1.0000000000000000000000000000000000000000000000000000000000000000000000000000000000000\
00000000000000

FIG. 3: Hypergeometric formula $P(\alpha)$ for Hilbert-Schmidt generic 2×2 *generalized* separability probabilities and evidence that it reproduces the basic three (real $[\alpha = \frac{1}{2}]$, complex $[\alpha = 1]$ and quaternionic $[\alpha = 2]$) conjectures of $\frac{29}{64}$, $\frac{8}{33}$ and $\frac{26}{323}$

II. RESULTS

A. The three basic conjectures revisited

1. $\alpha = \frac{1}{2}$–the two-rebit case

In [1], a lower-bound estimate of the two-rebit separability probability was obtained, with the use of the first 3,310 moments of $|\rho^{PT}|$. It was 0.999955 times as large as $\frac{29}{64} \approx 0.453120$. With the use, now, of 7,501 moments, the figure increases to 0.999989567. This outcome, thus, fortifies our previous conjecture.

2. $\alpha = 1$–the two-qubit case

In [1], a lower-bound estimate of the two-qubit separability probability was obtained, with the use of the first 2,415 moments of $|\rho^{PT}|$, that was 0.999997066 times as large as $\frac{8}{33} \approx 0.242424$ (cf. [25, eq. (B7)]). Employing 7,501 moments, this figure increases to 0.99999986.

3. $\alpha = 2$–the quaternionic case

In [1], a lower-bound estimate of the (presumptive) quaternionic separability probability was obtained that was 0.999999987 times as large as $\frac{26}{323} \approx 0.0804954$, using the first 2,325 moments of $|\rho^{PT}|$. Based on 7,501 moments, this figure increases, quite remarkably still, to 0.999999999936.

B. Generalized separability probability formula

A principal motivation in undertaking the analyses reported here–in addition, to further scrutinizing the three specific conjectures reported in [1]–was to uncover the functional relation underlying the curve in Fig. 1 (and/or its original non-logarithmic counterpart).

Preliminarily, let us note that the *zeroth*-order approximation (being independent of the particular value of α) provided by the Provost probability-distribution-reconstruction algorithm is simply the *uniform* distribution over the interval $[-\frac{1}{16}, \frac{1}{256}]$. The corresponding

zeroth-order separability probability estimate is the cumulative probability of this distribution over the nonnegative subinterval $[0, \frac{1}{256}]$, that is, $\frac{1}{256}/(\frac{1}{16}+\frac{1}{256}) = \frac{1}{17} \approx 0.0588235$. So, it certainly appears that speedier convergence (sec. II A) of the algorithm occurs for separability probabilities, the true values of which are initially close to $\frac{1}{17}$ (such as $\frac{26}{323} \approx 0.0804954$ in the quaternionic case). Convergence also markedly increases as α increases.

It appeared, numerically, that the generalized separability probabilities for integral and half-integral values of α were rational values (not only $\frac{29}{64}, \frac{8}{33}, \frac{26}{323}$, for the three specific values $\alpha = \frac{1}{2}, 1, 2$ of original focus). With various computational tools and search strategies based upon emerging mathematical properties, we were able to advance additional, seemingly plausible conjectures as to the exact values for $\alpha = 3, 4, \ldots, 32$, as well. (We inserted many of our high-precision numerical estimates into the search box on the Wolfram Alpha website–which then indicated likely candidates for corresponding rational values.)

We fed this sequence of thirty-two conjectured rational numbers into the FindSequenceFunction command of Mathematica. (This command "attempts to find a simple function that yields the sequence a_i when given successive integer arguments," but apparently can succeed with rational arguments, as well.) To our considerable satisfaction, this produced a generating formula (incorporating a diversity of hypergeometric functions of the ${}_pF_{p-1}$ type, $p = 7, \ldots, 11$, *all* with argument $z = \frac{27}{64} = (\frac{3}{4})^3$) for the sequence. (Let us note that $z^{-\frac{1}{2}} = \sqrt{\frac{64}{27}}$ is the "residual entropy for square ice" [28, p. 412] (cf. [29, eqs.[(27), (28)]. An analogous appearance of $\frac{27}{64}$ occurs in a hypergeometric ["Ramanujan-like"] summation for $\frac{16\pi^2}{3}$ [30] of Guillera. In a related email he wrote: "Some values of "z", for example z = 27 / 64 appear frequently in hypergeometric identities. I think it is due to a "modular" or a "modular-like" origin."). In fact, the Mathematica command succeeds using only the first twenty-eight conjectured rational numbers, but no fewer–so it seems fortunate, our computations were so extensive.)

However, the formula produced by the Mathematica command was quite cumbersome in nature (extending over several pages of output). With its use, nevertheless, we were able to convincingly generate rational values for *half*-integral α (including the two-rebit $\frac{29}{64}$ conjecture), also fitting our corresponding half-integral thirty-two numerical estimates exceedingly well. (Let us strongly emphasize that the hypergeometric-based formula was generated using *only* the integral values of α. The process was fully reversible, and we could first employ the half-integral results to generate the formula–which then–seemingly perfectly

fitted the integral values.)

At this point, for illustrative purposes, let us list the first ten half-integral and ten integral rational values (generalized separability probabilities), along with their approximate numerical values.

$$
\begin{array}{ll}
\alpha = \frac{1}{2} \; \frac{29}{64} \; 0.453125 & \alpha = 1 \; \frac{8}{33} \; 0.242424 \\
\alpha = \frac{3}{2} \; \frac{36061}{262144} \; 0.137562 & \alpha = 2 \; \frac{26}{323} \; 0.0804954 \\
\alpha = \frac{5}{2} \; \frac{51548569}{1073741824} \; 0.0480083 & \alpha = 3 \; \frac{2999}{103385} \; 0.0290081 \\
\alpha = \frac{7}{2} \; \frac{38911229297}{2199023255552} \; 0.0176948 & \alpha = 4 \; \frac{44482}{4091349} \; 0.0108722 \\
\alpha = \frac{9}{2} \; \frac{60515043681347}{9007199254740992} \; 0.00671852 & \alpha = 5 \; \frac{89514}{21460999} \; 0.00417101 \\
\alpha = \frac{11}{2} \; \frac{71925602948804923}{27670116110564327424} \; 0.0025994 & \alpha = 6 \; \frac{179808469}{110638410169} \; 0.00162519 \\
\alpha = \frac{13}{2} \; \frac{33873748333673072336269}{33245460039402302304419 84} \; 0.0010189 & \alpha = 7 \; \frac{191151001}{298529164591} \; 0.000640309 \\
\alpha = \frac{15}{2} \; \frac{124792688228667229196729}{309485009821345068724781056} \; 0.000403227 & \alpha = 8 \; \frac{1331199762}{5232880523393} \; 0.000254391 \\
\alpha = \frac{17}{2} \; \frac{407557367133399293946182513}{2535301200456458802993406410752} \; 0.000160753 & \alpha = 9 \; \frac{74195568677}{729345064647247} \; 0.000101729 \\
\alpha = \frac{19}{2} \; \frac{1338799759394288468677657208071}{20769187434139310514121985316880384} \; 0.0000644609 & \alpha = 10 \; \frac{730710456538}{17868447453498669} \; 0.0000408939
\end{array} \tag{1}
$$

To simplify the cumbersome (several-page) output yielded by the Mathematica FindSequenceFunction command, we employed certain of the "contiguous rules" for hypergeometric functions listed by C. Krattenthaler in his package HYP [31] (cf. [32]). Multiple applications of the rules C14 and C18 there, together with certain gamma function simplifications suggested by C. Dunkl, led to the rather more compact formula displayed in Fig. 3. This formula incorporates a six-member family ($k = 1, \ldots, 6$) of ${}_7F_6$ hypergeometric functions, differing only in the first upper index k,

$$
{}_7F_6\left(k, \alpha+\frac{2}{5}, \alpha+\frac{3}{5}, \alpha+\frac{4}{5}, \alpha+\frac{5}{6}, \alpha+\frac{7}{6}, \alpha+\frac{6}{5}; \alpha+\frac{13}{10}, \alpha+\frac{3}{2}, \alpha+\frac{17}{10}, \alpha+\frac{19}{10}, \alpha+2, \alpha+\frac{21}{10}; \frac{27}{64}\right). \tag{2}
$$

(The reader will note interesting sequences of upper and lower parameters (cf. [33]).) We are only able to, in general, evaluate the formula numerically, but then to arbitrarily high (hundreds, if not thousand-digit) precision, giving us strong confidence in the validity of the *exact* generalized separability probabilities that we advance.

Let us now apply the formula (Fig. 3) to values of α other than the basic sixty-four. For $\alpha = 0$, the formula yields–as would be expected–the "classical separability probability" of 1.

Further, proceeding in a purely formal manner (since there appears to be no corresponding genuine probability distribution over $[-\frac{1}{16}, \frac{1}{256}]$), for the *negative* value $\alpha = -\frac{1}{2}$, the formula yields $\frac{2}{3}$. For $\alpha = -\frac{1}{4}$, it gives -2. Remarkably still, for $\alpha = \frac{1}{4}$, the result is clearly (to one thousand decimal places) equal to $2 - \frac{34}{21\text{agm}\left(1,\sqrt{2}\right)} = 2 - \frac{17\Gamma\left(\frac{1}{4}\right)^2}{21\sqrt{2}\pi^{3/2}} \approx 0.6486993992$, where the arithmetic-geometric mean of 1 and $\sqrt{2}$ is indicated. (The reciprocal of this mean is Gauss's constant.) For $\alpha = \frac{3}{4}$, the result equals $2 - \frac{9689\Gamma\left(\frac{3}{4}\right)}{4420\sqrt{\pi}\Gamma\left(\frac{5}{4}\right)} \approx 0.3279684732$, while for $\alpha = -\frac{3}{4}$, we have $\frac{128}{21\text{agm}\left(1,\sqrt{2}\right)} + 2 = 2 + \frac{32\sqrt{2}\Gamma\left(\frac{1}{4}\right)^2}{21\pi^{3/2}} \approx 7.087249321$. For $\alpha = \frac{2}{3}$, the outcome is $2 - \frac{288927\Gamma\left(\frac{1}{3}\right)^3}{344080\pi^2} \approx 0.36424897456$. Results are presented in the table

$$\begin{pmatrix} \alpha & P(\alpha) & \text{value} \\ -\frac{3}{4} & 2 + \frac{32\sqrt{2}\Gamma\left(\frac{1}{4}\right)^2}{21\pi^{3/2}} & 7.08725 \\ -\frac{2}{3} & 2 - \frac{8\pi}{\sqrt{3}\Gamma\left(\frac{1}{3}\right)^3} & 1.24527 \\ -\frac{1}{2} & \frac{2}{3} & 0.666667 \\ -\frac{1}{3} & 2 + \frac{3\Gamma\left(\frac{1}{3}\right)^3}{4\pi^2} & 3.461 \\ -\frac{1}{4} & 2 & 2 \\ \frac{1}{4} & 2 - \frac{17\Gamma\left(\frac{1}{4}\right)^2}{21\sqrt{2}\pi^{3/2}} & 0.648699 \\ \frac{1}{3} & 2 - \frac{459\sqrt{3}\pi}{91\Gamma\left(\frac{1}{3}\right)^3} & 0.572443 \\ \frac{2}{3} & 2 - \frac{288927\Gamma\left(\frac{1}{3}\right)^3}{344080\pi^2} & 0.364249 \\ \frac{3}{4} & 2 - \frac{9689\Gamma\left(\frac{3}{4}\right)}{4420\sqrt{\pi}\Gamma\left(\frac{5}{4}\right)} & 0.327968 \end{pmatrix}. \tag{3}$$

(Let us note that the term $\frac{3\Gamma\left(\frac{1}{3}\right)^3}{4\pi^2} \approx 1.46099848$ present in the result for $\alpha = -\frac{1}{3}$ is "Baxter's four-coloring constant" for a triangular lattice [28, p. 413].) Also, for $\alpha = -1$, we have $\frac{2}{5}$. For $\alpha = -\frac{3}{2}$, the result is $\frac{2}{3}$.

III. CONCISE FORMULATION OF HYPERGEOMETRIC EXPRESSION

The concise formulation of $P(\alpha)$ takes the form (Fig. 4)

$$P(\alpha) = \Sigma_{i=0}^{\infty} f(\alpha + i), \tag{4}$$

where

$$f(\alpha) = P(\alpha) - P(\alpha+1) = \frac{q(\alpha) 2^{-4\alpha-6}\Gamma(3\alpha + \frac{5}{2})\Gamma(5\alpha+2)}{3\Gamma(\alpha+1)\Gamma(2\alpha+3)\Gamma(5\alpha + \frac{13}{2})}, \tag{5}$$

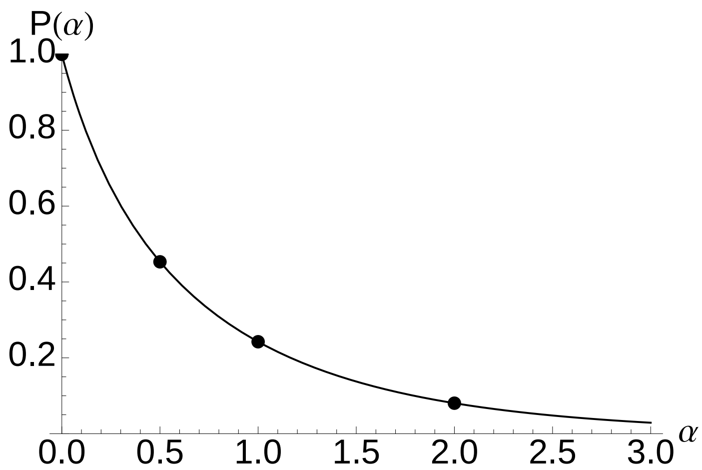

FIG. 4: Generalized two-qubit separability probability function $P(\alpha)$, with $P(0) = 1, P(\frac{1}{2}) = \frac{29}{64}, P(1) = \frac{8}{33}, P(2) = \frac{26}{323}$ for generic classical four-level ($\alpha = 0$), two-rebit ($\alpha = \frac{1}{2}$), two-qubit ($\alpha = 1$) and two-quaterbit ($\alpha = 2$) systems, respectively.

and

$$q(\alpha) = 185000\alpha^5 + 779750\alpha^4 + 1289125\alpha^3 + 1042015\alpha^2 + 410694\alpha + 63000 = \tag{6}$$

$$\alpha(5\alpha(25\alpha(2\alpha(740\alpha + 3119) + 10313) + 208403) + 410694) + 63000.$$

We had previously ourselves been unable to find an equivalent form of $P(\alpha)$ with fewer than six hypergeometric functions [34, Fig. 3]. Qing-Hu Hou and colleagues of the Center for Combinatorics of Nankai University, however, were able to obtain the remarkably succinct and clearly correct results (4)-(6)–which they communicated to us in a few brief, informal e-mail messages. (They provided two Maple worksheets they employed [Figs. 5 and 6].) They, first, observed that the hypergeometric-based formula for $P(\alpha)$ could be expressed as an infinite summation. Letting $P_l(\alpha)$ be the l-th such summand, application of Zeilberger's algorithm [35] (a method for producing combinatorial identities, also known as "creative telescoping") yielded that

$$P_l(\alpha) - P_l(\alpha + 1) = -P_{l+1}(\alpha) + P_l(\alpha). \tag{7}$$

(The package APCI–available at http://www.combinatorics.net.cn/homepage/hou/–was employed. In a different quantum-information context, Datta employed the algorithm to ascertain that no closed form exists for a certain series, "retarding" the evaluation of the

ratio "of the negativity of random pure states to the maximal negativity for Haar-distributed states of n qubits [36, App. A].) Summing over l from 0 to ∞, Hou and colleagues found that

$$P(\alpha) - P(\alpha + 1) = P_0(\alpha). \tag{8}$$

Letting $f(\alpha) = P_0(\alpha)$, the concise summation formula (4) is obtained. (C. Krattenthaler indicated–and Hou agreed–that these results might equally well be derived without recourse to Zeilberger's algorithm. Also, a referee expressed puzzlement at the peculiar form of eq. (7). This appears to be an artifact arising from the particular manner in which the algorithm is applied in the proving of hypergeometric identities.)

```
> with(APCI);
```

[AbelZ, Dis_set, Ext_Zeil, Gosper, Zeil, hyper_simp, hyperterm, poch, qExt_Zeil, qGosper, qZeil, qhyper_simp, qhyperterm, qpoch] **(1)**

```
> t:=hyperterm([k,a+2/5,a+3/5,a+4/5,a+5/6,a+7/6,a+6/5],[a+13/10,
  a+3/2,a+17/10,a+19/10,a+2,a+21/10],27/64,l);
```

$$t := \left(\mathrm{pochhammer}(k, l)\,\mathrm{pochhammer}\left(a+\frac{2}{5}, l\right)\mathrm{pochhammer}\left(a+\frac{3}{5}, l\right)\mathrm{pochhammer}\left(a+\frac{4}{5}, l\right)\mathrm{pochhammer}\left(a+\frac{5}{6}, l\right)\mathrm{pochhammer}\left(a+\frac{7}{6}, l\right)\mathrm{pochhammer}\left(a+\frac{6}{5}, l\right)\left(\frac{27}{64}\right)^{l}\right) \Big/ \left(\mathrm{pochhammer}\left(a+\frac{13}{10}, l\right)\mathrm{pochhammer}\left(a+\frac{3}{2}, l\right)\mathrm{pochhammer}\left(a+\frac{17}{10}, l\right)\mathrm{pochhammer}\left(a+\frac{19}{10}, l\right)\mathrm{pochhammer}(a+2, l)\,\mathrm{pochhammer}\left(a+\frac{21}{10}, l\right) l!\right) \quad \textbf{(2)}$$

```
> PP:=(a*(5*a*(25*a*(2*a*(740*a-581)+161)+628)+39)-54)*subs(k=1,t)+
  (5*a*(25*a*(8*a*(925*a-2431)+22255)-312019)+347274)*subs(k=2,t)
  +10*( (25*a*(4*a*(3700*a-12843)+66227)-769797)*subs(k=3,t)+75*(
  (8*a*(1850*a-6131)+44133)*subs(k=4,t) + 8*( (3700*a-7981)*subs(k=
  5,t) + 3700*subs(k=6,t) ) ) ):
> Pl:=4^(-2*a-3)*GAMMA(3*a+5/2)*GAMMA(5*a+2)/3/GAMMA(a+1)/GAMMA(2*
  a+3)/GAMMA(5*a+13/2)*PP:
```

```
> re:=Zeil(Pl,a,l,`cert`);
```

$$re := [S(a) - S(a+1) = 0, -1] \quad \textbf{(3)}$$

```
> f:=-factor(hyper_simp( subs(l=0,Pl*re[2]) ));
```

$$f := \frac{1}{3}\,\frac{1}{a!\,(2a+2)!\left(5a+\frac{11}{2}\right)!}\left(\left(185000\,a^5 + 779750\,a^4 + 1289125\,a^3 + 1042015\,a^2 + 410694\,a + 63000\right)2^{-4a-6}\left(3a+\frac{3}{2}\right)!\,(5a+1)!\right) \quad \textbf{(4)}$$

```
> add(evalf(hyper_simp(subs(a=1/4+i, f))), i=0..30);
```

0.6486993992 **(5)**

```
> add(evalf(hyper_simp(subs(a=-1+i, f))), i=0..30);
```

-2.000000001 **(6)**

```
> add(evalf(hyper_simp(subs(a=i, f))), i=0..30);
```

0.9999999999 **(7)**

FIG. 5: First Maple worksheet of Hou used in deriving concise form of hypergeometric formula

```
> with(APCI);
```
$$[AbelZ, Dis\_set, Ext\_Zeil, Gosper, Zeil, hyper\_simp, hyperterm, poch, qExt\_Zeil, qGosper, qZeil, qhyper\_simp, qhyperterm, qpoch] \quad (1)$$

```
> t:=hyperterm([k,a+2/5,a+3/5,a+4/5,a+5/6,a+7/6,a+6/5],[a+13/10,
a+3/2,a+17/10,a+19/10,a+2,a+21/10],27/64,l);
```
$$t := \left(\mathrm{pochhammer}(k, l)\,\mathrm{pochhammer}\left(a+\frac{2}{5}, l\right)\mathrm{pochhammer}\left(a+\frac{3}{5}, l\right)\mathrm{pochhammer}\left(a+\frac{4}{5}, l\right)\mathrm{pochhammer}\left(a+\frac{5}{6}, l\right)\mathrm{pochhammer}\left(a+\frac{7}{6}, l\right)\mathrm{pochhammer}\left(a+\frac{6}{5}, l\right)\left(\frac{27}{64}\right)^{l}\right) \Big/ \left(\mathrm{pochhammer}\left(a+\frac{13}{10}, l\right)\mathrm{pochhammer}\left(a+\frac{3}{2}, l\right)\mathrm{pochhammer}\left(a+\frac{17}{10}, l\right)\mathrm{pochhammer}\left(a+\frac{19}{10}, l\right)\mathrm{pochhammer}(a+2, l)\,\mathrm{pochhammer}\left(a+\frac{21}{10}, l\right) l!\right) \quad (2)$$

```
> PP:=(a*(5*a*(25*a*(2*a*(740*a-581)+161)+628)+39)-54)*subs(k=1,t)+
(5*a*(25*a*(8*a*(925*a-2431)+22255)-312019)+347274)*subs(k=2,t)
+10*( (25*a*(4*a*(3700*a-12843)+66227)-769797)*subs(k=3,t)+75*(
(8*a*(1850*a-6131)+44133)*subs(k=4,t) + 8*( (3700*a-7981)*subs(k=
5,t) + 3700*subs(k=6,t) ) ) ):
```

```
> P1:=4^(-2*a-3)*GAMMA(3*a+5/2)*GAMMA(5*a+2)/3/GAMMA(a+1)/GAMMA(2*
a+3)/GAMMA(5*a+13/2)*PP:
```

```
> re:=Zeil(P1,a,l,`cert`);
```
$$re := [S(a) - S(a+1) = 0, -1] \quad (3)$$

```
> zz:=-factor(hyper_simp( subs(l=0,P1*re[2]) ));
```
$$zz := \frac{1}{3}\,\frac{1}{a!\,(2a+2)!\left(5a+\frac{11}{2}\right)!}\left((185000a^5+779750a^4+1289125a^3+1042015a^2+410694a+63000)\,2^{-4a-6}\left(3a+\frac{3}{2}\right)!\,(5a+1)!\right) \quad (4)$$

The ratio of two consecutive terms

```
> r1:=hyper_simp(subs(l=l+1,P1)/P1);
```
$$r1 := (3\,(3769584+10406099a+10406099l+1704750a^4+11437890a^2+6258125a^3+185000a^5+925000a^4l+6819000a^3l+18774375a^2l+22875780al+1850000a^3l^2+10228500a^2l^2+18774375al^2+11437890l^2+1850000a^2l^3+6819000al^3+6258125l^3+925000al^4+1704750l^4+185000l^5)\,(5a+2+5l)\,(5a+3+5l)\,(5a+4+5l)\,(6a+5+6l)\,(6a+7+6l)\,(5a+6+5l))\Big/(8\,(10a+21+10l)\,(a+2+l)\,(10a+19+10l)\,(10a+17+10l)\,(2a+3+2l)\,(10a+13+10l)\,(63000+410694a+410694l+779750a^4+1042015a^2+1289125a^3+185000a^5+925000a^4l+3119000a^3l+3867375a^2l+2084030al+1850000a^3l^2+4678500a^2l^2+3867375al^2+1042015l^2+1850000a^2l^3+3119000al^3+1289125l^3+925000al^4+779750l^4+185000l^5)) \quad (5)$$

$$)$$

```
> r2:=hyper_simp(subs(a=a+l+1,zz)/subs(a=a+l,zz));
```

$$r2 := \left(3 \left(3769584 + 10406099\,a + 10406099\,l + 1704750\,a^4 + 11437890\,a^2 + 6258125\,a^3 + 185000\,a^5 + 925000\,a^4\,l + 6819000\,a^3\,l + 18774375\,a^2\,l + 22875780\,a\,l + 1850000\,a^3\,l^2 + 10228500\,a^2\,l^2 + 18774375\,a\,l^2 + 11437890\,l^2 + 1850000\,a^2\,l^3 + 6819000\,a\,l^3 + 6258125\,l^3 + 925000\,a\,l^4 + 1704750\,l^4 + 185000\,l^5\right) (5\,a + 2 + 5\,l)\,(5\,a + 3 + 5\,l)\,(5\,a + 4 + 5\,l)\,(6\,a + 5 + 6\,l)\,(6\,a + 7 + 6\,l)\,(5\,a + 6 + 5\,l)\right) \Big/ \left(8\,(10\,a + 21 + 10\,l)\,(a + 2 + l)\,(10\,a + 19 + 10\,l)\,(10\,a + 17 + 10\,l)\,(2\,a + 3 + 2\,l)\,(10\,a + 13 + 10\,l)\left(63000 + 410694\,a + 410694\,l + 779750\,a^4 + 1042015\,a^2 + 1289125\,a^3 + 185000\,a^5 + 925000\,a^4\,l + 3119000\,a^3\,l + 3867375\,a^2\,l + 2084030\,a\,l + 1850000\,a^3\,l^2 + 4678500\,a^2\,l^2 + 3867375\,a\,l^2 + 1042015\,l^2 + 1850000\,a^2\,l^3 + 3119000\,a\,l^3 + 1289125\,l^3 + 925000\,a\,l^4 + 779750\,l^4 + 185000\,l^5\right)\right) \qquad \textbf{(6)}$$

```
> normal( r1-r2 );
```

$$0 \qquad \textbf{(7)}$$

FIG. 6: Second Maple worksheet of Hou used in deriving concise form of hypergeometric formula (Fig. 2)

We certainly need to indicate, however, that if we do explicitly perform the infinite summation indicated in (4), then we revert to a (”nonconcise”) form of $P(\alpha)$, again containing six hypergeometric functions. Further, it appears that we can only evaluate (4) numerically–but then easily to hundreds and even thousands of digits of precision–giving us extremely high confidence in the specific rational-valued Hilbert-Schmidt separability probabilities advanced.

There remain the important problems of formally verifying the formulas for $P(\alpha)$ (as well as the underlying determinantal moment formulas in [1], employed in the probability-distribution reconstruction process), and achieving a better understanding of what these results convey regarding the geometry of quantum states [16, 37, 38]. Further, questions of the asymptotic behavior of the formula ($\alpha \to \infty$) and of possible Bures metric [3, 4, 6, 16, 39] counterparts to it, are under investigation [40]. Also, we are presently engaged in attempting to determine further properties–in addition to the cumulative (separability) probability over $[0, \frac{1}{256}]$–of the probability distributions of $|\rho^{PT}|$ over $[-\frac{1}{16}, \frac{1}{256}]$, as a function of the Dyson-index-like parameter α. As one finding in this direction, it appears that the y-intercept (at which $|\rho^{PT}| = 0$) in the presumed quaternionic case ($\alpha = 2$) is $\frac{7425}{34} = \frac{3^3 \times 5^2 \times 11}{2 \times 17}$. (The Legendre-polynomial-based probability-distribution reconstruction algorithm of Provost [18] yielded an estimate 0.99999999742 times as large as $\frac{7425}{34}$, when implemented with 10,000 moments. Based also on 10,000 moments, the two-qubit [$\alpha = 1$] counterpart was estimated as 389.994942076.)

The foundational paper of Życzkowski, Horodecki, Sanpera and Lewenstein,”Volume of the set of separable states” [2], did ask for *volumes*, not specifically *probabilities*. At least, for the two-rebit, two-qubit and two-quaterbit cases, $\alpha = \frac{1}{2}, 1$ and 2, we can readily convert the corresponding separability probabilities to the separable volumes $\frac{29\pi^4}{61931520} = \frac{29\pi^4}{2^{16} \cdot 3^3 \cdot 5 \cdot 7}$, $\frac{\pi^6}{449513064000} = \frac{\pi^6}{2^6 \cdot 3^6 \cdot 5^3 \cdot 7^2 \cdot 11^2 \cdot 13}$ and $\frac{\pi^{12}}{3914156909371803494400000} = \frac{\pi^{12}}{2^{14} \cdot 3^{10} \cdot 5^5 \cdot 7^3 \cdot 11^2 \cdot 13 \cdot 17^2 \cdot 19^2 \cdot 23}$, using the Hilbert-Schmidt volume formulas of Andai [26, Thms. 1-3] (cf. [15, 16]). The determination of separable volumes–as opposed to probabilities–for other values of α than these three appears to be rather problematical, however.

Let us also note that Theorem 2 of [41], in conjunction with the results here, allows us to immediately obtain the separability probabilities of the generic minimally-degenerate/boundary 8-, 14-, and 26-dimensional two-rebit, two-qubit, and two-quaterbit states, as one-half (that is, $\frac{29}{128}, \frac{4}{33}$ and $\frac{13}{323}$) the separability probabilities of their generic

non-degenerate counterparts.

IV. APPENDIX–EXACT VALUES OF DERIVATIVES OF $P(\alpha)$

A. Succeeding deriviatives at $\alpha = 0$

The first derivative of $P(\alpha)$ evaluated at (the classical case) $\alpha = 0$ is -2, while the second derivative is $40 - 20\zeta(2) = 40 - \frac{10\pi^2}{3} \approx 7.10132$. (The third derivative was computed as -43.7454236566749417600.)

B. First derivatives at $\alpha = 1, 2 \ldots$, *et al*

The first derivative of $P(\alpha)$ at $\alpha = -\frac{1}{2}$ is $-\frac{80}{3}$ and at $\alpha = \frac{1}{2}$ is $\frac{1}{384}(917 - 984\log(2)) \approx 0.611831$, and -2 at $\alpha = 0$, as previously mentioned. We have also been able to determine rational values of $P(\alpha)$ for $\alpha = 1, 2, \ldots, 97$. We list the first seven of these. (The Mathematica command FindSequenceFunction, however, did not succeed in this instance in generating an underlying function for this sequence of 97 rational numbers–although, of course, one can be directly obtained from our explicit forms above of $P(\alpha)$).

$$\begin{pmatrix} \alpha & P'(\alpha) \\ 1 & -\frac{130577}{457380} \approx -0.285489 \\ 2 & -\frac{3177826243}{37595998440} \approx -0.0845257 \\ 3 & -\frac{3598754002551529}{124409677632540300} \approx -0.0289266 \\ 4 & -\frac{943222153906869801499}{89625168823088671652880} \approx -0.0105241 \\ 5 & -\frac{774586890593597806387 1447}{19561350296052597373545204 00} \approx -0.00395978 \\ 6 & -\frac{163704960709243940550573265691777}{107569184582725029279135417408286275} \approx -0.00152186 \\ 7 & -\frac{1245552750715798766420577238084757 61407}{2098676284852549317327092942719623 33917400} \approx -0.000593494 \end{pmatrix}. \tag{9}$$

Acknowledgments

I would like to express appreciation to the Kavli Institute for Theoretical Physics (KITP) for computational support in this research, and to Christian Krattenthaler, Charles F. Dunkl,

Michael Trott, Jorge Santos, and Qing-Hu Hou and his colleagues for their expert advice.

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